

## Entanglement entropies in conformal systems with boundaries

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We study the entanglement entropies in one-dimensional open critical systems, whose effective description is given by a conformal field theory with boundaries. We show that, for pure-state systems formed by the ground state or by the excited states associated to primary fields, the entanglement entropies have a finite-size behavior that depends on the correlation of the underlying field theory. The analytical results are checked numerically, finding excellent agreement for the quantum chains ruled by the theories with central charge  $c = 1/2$  and 1.

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In recent years there has been a flurry of activity devoted to characterize quantum many-body systems and quantum field theories using the concept of entanglement (see Ref. 1 and references therein for a review). Under certain conditions, the low-energy states of local Hamiltonians satisfy an entropic area law, according to which the entanglement entropy (EE) of a subsystem is proportional to the area of its boundary.<sup>2</sup> In one spatial dimension, violations to this area law appear if the system is gapless and described by a conformal field theory (CFT):<sup>3,4</sup> in this case, the ground-state (GS) EE grows with the log of the subsystem size.<sup>5-7</sup> On the other hand, it is well known that the dominant finite-size correction to the GS energy of critical systems is related to the central charge  $c$ .<sup>8</sup> A similar correspondence also exists between the central charge and the Rényi entanglement entropies (REE's) of the GS.<sup>5-7</sup> In the same vein, we would expect that the scaling dimensions of the primary operators are related with the REE's of the excited states (ES's), since the finite mass gaps of critical lattice Hamiltonians are also related with them.<sup>8</sup> Indeed, this latter correspondence was proven recently for conformal systems with *periodic* boundary conditions.<sup>9,10</sup> The main result of these works is that the  $n$ th REE is given in terms of the  $2n$ -point correlator of the corresponding primary field placed at special positions depending on the subsystem size.

In this letter we shall generalize this result to *open* lattice Hamiltonians, effectively described by boundary conformal field theory (BCFT).<sup>11</sup> BCFT has a wide range of applications to impurity problems,<sup>12</sup> string theory,<sup>13</sup> etc., which justifies the generalization pursued here. Moreover, the generalization is, as we shall see, nontrivial, since BCFT has a very rich mathematical structure, which is worth analyzing from the entanglement point of view. Apart from these many reasons of interest, it is worth citing that the problem is quite long standing,<sup>14,15</sup> and our work represents its final solution.

We shall start with some basic definitions. The REE's are defined as follows:

$$S_n \equiv \frac{1}{1-n} \ln \text{Tr}_A \rho_A^n, \quad (1)$$

where  $n$  is a positive real,  $\rho_A$  is the reduced density matrix of a subsystem  $A$ , and the trace is over the  $A$ 's Hilbert space. If  $\rho_A$  is constructed from the GS of a CFT, one has<sup>7</sup>

$$S_n^{\text{CFT}}(l, L) = c_n^n + \frac{c}{3\eta} \left(1 + \frac{1}{n}\right) \ln \left[ \frac{\eta L}{\pi} \sin \frac{\pi l}{L} \right], \quad (2)$$

where  $l$  is the size of  $A$ ,  $L$  is the total-system size, and  $\eta = 1, 2$  for periodic boundary conditions (PBC's) or free boundary conditions (FBC's);  $c$  is the central charge and  $c_n^n$  is a constant that depends on the BC's.<sup>4</sup> For open systems,  $l$  is measured from the left edge. Equation (2) may have significant corrections which carry useful information about the underlying CFT.<sup>16-18</sup> A different kind of corrections arises when, instead of considering the GS, one looks at the ES's,<sup>9,10,19,20</sup> or when the system satisfies general BC's preserving its conformal invariance (FBC's are just one of them).<sup>14,15</sup> In particular, the corrections in this last case have, up to now, not been derived analytically, and their knowledge would be a great advance, both from a practical and a conceptual point of view. In the following, we present the general CFT framework allowing the analytical computation of such corrections. These results are then verified with density-matrix renormalization group (DMRG) calculations in two examples: the  $c = 1/2$  minimal CFT and the  $c = 1$  massless compactified free boson.

Let us consider a one-dimensional (1D) conformal system, defined on a strip of width  $L$ . Cardy<sup>11</sup> showed the existence of BC's, denoted as  $\{\tilde{\alpha}\}$ , that preserve the conformal invariance, and such that the partition function takes the form

$$Z_{\tilde{\alpha}\tilde{\beta}}(q) = \sum_h \mathcal{N}_{\tilde{\alpha}\tilde{\beta}}^h \chi_h(q), \quad (3)$$

where  $q \equiv e^{-\pi\beta/L}$  (being  $\beta$  the inverse temperature),  $h$  are the conformal dimensions of the primary fields, and  $\chi_h$  are the associated characters. The integers  $\mathcal{N}_{\tilde{\alpha}\tilde{\beta}}^h$  are the fusion coefficients of the theory.<sup>3,4</sup> The derivation of the REE's of ES's, originating from the primary operator  $\Upsilon(w)$  for open conformal systems, follows closely the one of periodic

boundary conditions given in Ref. 9. The REE's are given by

$$S_n(l, L) = S_n^{\text{CFT}}(l, L) + \frac{1}{1-n} \ln F_\Upsilon^{(n)}, \quad (4)$$

$$F_\Upsilon^{(n)}(x) = \frac{\text{Tr}_A \rho_{A, \Upsilon}^n}{\text{Tr}_A \rho_{A, \text{GS}}^n},$$

where  $\rho_{A, \Upsilon}$  and  $\rho_{A, \text{GS}}$  are the reduced density matrices obtained from the ES produced by the primary field  $\Upsilon$  and from the GS, respectively. The ratio  $F_\Upsilon^{(n)}$  can be computed using path-integral methods.<sup>9</sup> We explain below the main steps of the derivation.

Let us first split the strip into the subsystems  $A = [0, l], B = [l, L]$ . This strip is parameterized by the complex coordinate  $w = \sigma + i\tau$ ,  $\sigma \in [0, L], \tau \in (-\infty, \infty)$ . We make the conformal transformation

$$\zeta = \frac{\sin \frac{\pi(w-l)}{2L}}{\sin \frac{\pi(w+l)}{2L}}, \quad (5)$$

which maps the strip into the unit disk  $\mathbb{D} = \{\zeta, |\zeta| \leq 1\}$ . The intervals  $A$  and  $B$  are mapped into the segments  $(-1, 0)$  and  $(0, 1)$ , respectively. The boundaries of the strip,  $\sigma = 0, L$ , are mapped into the boundary of the disk ( $|\zeta| = 1$ ), and the infinite past ( $w_\infty^- = -i\infty$ ) and infinite future ( $w_\infty^+ = i\infty$ ) are mapped into

$$w_\infty^- \rightarrow \zeta_\infty^- = e^{-i\pi x}, \quad w_\infty^+ \rightarrow \zeta_\infty^+ = e^{i\pi x}, \quad x \equiv \frac{l}{L}. \quad (6)$$

Next, we make  $n$  copies of the unit disk and sew them along the cut  $(-1, 0)$ , obtaining the Riemann surface  $\mathcal{R}_n$ , which can also be mapped into the unit disk by the conformal transformation

$$z = \zeta^{1/n} = \left( \frac{\sin \frac{\pi(w-l)}{2L}}{\sin \frac{\pi(w+l)}{2L}} \right)^{1/n}. \quad (7)$$

The points  $\zeta_\infty^\pm$  give rise to  $2n$  points on  $\mathcal{R}_n$ :

$$z_{k,n}^\pm = e^{\frac{i\pi}{n}(\pm x + 2k)}, \quad k = 0, 1, \dots, n-1, \quad (8)$$

where the primary field  $\Upsilon$  and its conjugate  $\Upsilon^\dagger$  are inserted. Repeating the same steps as in Ref. 9, we arrive at an expression for Eq. (4):

$$F_\Upsilon^{(n)}(x) = \frac{e^{i2\pi(n-1)h} \left\langle \prod_{k=0}^{n-1} \Upsilon(z_{n,k}^-) \Upsilon^\dagger(z_{n,k}^+) \right\rangle}{n^{2nh} \langle \Upsilon(z_{1,0}^-) \Upsilon^\dagger(z_{1,0}^+) \rangle^n}, \quad (9)$$

where we have assumed that  $\Upsilon$  is a chiral primary field with conformal dimension  $h$ . A similar formula holds for nonchiral fields. The correlators in Eq. (9) are computed on the unit disk for fields inserted at its boundary. These primary fields change the boundary conditions  $a$  and  $b$  on each edge of the strip:  $\Upsilon$  changes them from  $a$  to  $b$ , while  $\Upsilon^\dagger$  changes them from  $b$  to  $a$ . Hence the numerator of Eq. (9) is proportional to the partition function of a disk with  $2n$  segments where the boundary conditions  $a$  and  $b$  alternate.<sup>4</sup> Equation (9) constitutes the main result of the work, which we shall verify below for two models.

(1) The first model is the  $c = 1/2$  minimal CFT. This CFT contains three primary fields: the identity  $\mathbb{I}$  ( $h_{\mathbb{I}} = 0$ ), a Majorana fermion  $\chi$  ( $h_\chi = 1/2$ ), and a spin field

$\sigma$  ( $h_\sigma = 1/16$ ), whose fusion rules are

$$\begin{aligned} \mathcal{N}_{00}^h &= \mathcal{N}_{\frac{1}{2}\frac{1}{2}}^h = \delta_0^h, & \mathcal{N}_{0\frac{1}{2}}^h &= \delta_{\frac{1}{2}}^h, \\ \mathcal{N}_{0\frac{1}{16}}^h &= \mathcal{N}_{\frac{1}{16}\frac{1}{2}}^h = \delta_{\frac{1}{16}}^h, & \mathcal{N}_{\frac{1}{16}\frac{1}{16}}^h &= \delta_0^h + \delta_{\frac{1}{2}}^h. \end{aligned} \quad (10)$$

This CFT describes the long-distance properties of the critical Ising model in a transverse field whose lattice Hamiltonian is

$$H_I = -\frac{1}{2} \sum_{j=1}^{L-1} \sigma_j^x \sigma_{j+1}^x - \frac{1}{2} \sum_{j=1}^L \sigma_j^z, \quad (11)$$

where  $\sigma^{x,y,z}$  are the Pauli matrices. The correspondence between the conformal BC's  $\{\tilde{\alpha}\}$  and the lattice BC's is the following:  $\tilde{0}$  ( $\frac{1}{2}$ ) corresponds to fix  $\sigma_{1,L}^x$  to  $+1$  ( $-1$ ), while  $\frac{1}{16}$  corresponds to free BC's.<sup>11,14</sup> For simplicity, we shall denote  $\tilde{0}, \frac{1}{2}, \frac{1}{16}$  by  $+, -, F$ .

We begin by considering the REE's of the GS with  $FF$  BC's (the two  $F$ 's refer to free BC's on both edges). The spin Hamiltonian Eq. (11) can be mapped into a free fermion Hamiltonian,<sup>21</sup> which we use to compute, by using the method of Ref. 22, the von Neumann entropy, i.e., the  $n = 1$  REE, for chains with lengths 60–180 in multiples of 20 (these will be the sizes considered in the rest of the work).

Using Eq. (2), and finite-size scaling (FSS) techniques, we obtain the asymptotic values  $c = 0.499$  and  $c_1^{\eta=2} = 0.241$ . The value of  $c$  agrees to high precision with the central charge of the critical Ising model.

Moreover, the value of  $c_1^{\eta=2}$  is very close to  $c_1^{\eta=1}/2$ , that can be obtained with PBC's. The relation  $c_1^{\eta=2} - c_1^{\eta=1}/2 = \ln g^{7,14}$  is satisfied in this case, because the boundary entropy (BE)  $\ln g$  vanishes for  $FF$  BC's.<sup>23</sup> Moreover, as a different reliability check, we verified that the REE's in this case are exactly one half of the ones of a spin-1/2 XX chain with  $FF$  BC's (see below), according to Ref. 24.

We next study the  $++$ BC's case (that is equivalent to  $--$ BC's). The fusion rule  $\mathcal{N}_{00}^h = \delta_0^h$  leads us to consider only the case in which  $h = 0$ , for which no corrections arise (apart, as we shall see, from constant BE contributions). We compute the REE's for the Hamiltonian Eq. (11) using the DMRG method<sup>25</sup> with up to 800 states per block, and three sweeps, which yields a truncation error of  $10^{-12}$  or less. Figures 1(a) and 1(b) display the results for  $n = 2, 3$  REE's: the data progressively flatten to the theoretical value  $-\frac{1}{2} \ln 2$ .<sup>14,26</sup> The convergence to the CFT predictions is of order  $10^{-3}$  or less, as confirmed by a FSS analysis [Fig. 1(i)]. This behavior can be ascribed to the presence of a slowly  $L$ -depending finite-size correction,<sup>24</sup> previously observed, for the Ising model, in Ref. 10.

We now consider the  $FBC$ 's case. The fusion rule  $\mathcal{N}_{\sigma\sigma}^\chi = 1$  implies that the first ES is generated by the primary field  $\chi$ . The associated  $F$  function is given by  $F_\chi^{(n)} = \sqrt{F_{i\partial\phi}^{(n)}}$ , where  $\phi$  is a massless free boson with  $c = 1$ .<sup>10</sup>

Quite interestingly,  $F_{i\partial\phi}^{(n)}$  has a general expression valid for any value of  $n > 0$ :<sup>27</sup>

$$F_{i\partial\phi}^{(n)}(x) = \left\{ \left[ \frac{2 \sin(\pi x)}{n} \right]^n \frac{\Gamma\left(\frac{1+n+n \csc(\pi x)}{2}\right)}{\Gamma\left(\frac{1-n+n \csc(\pi x)}{2}\right)} \right\}^2. \quad (12)$$

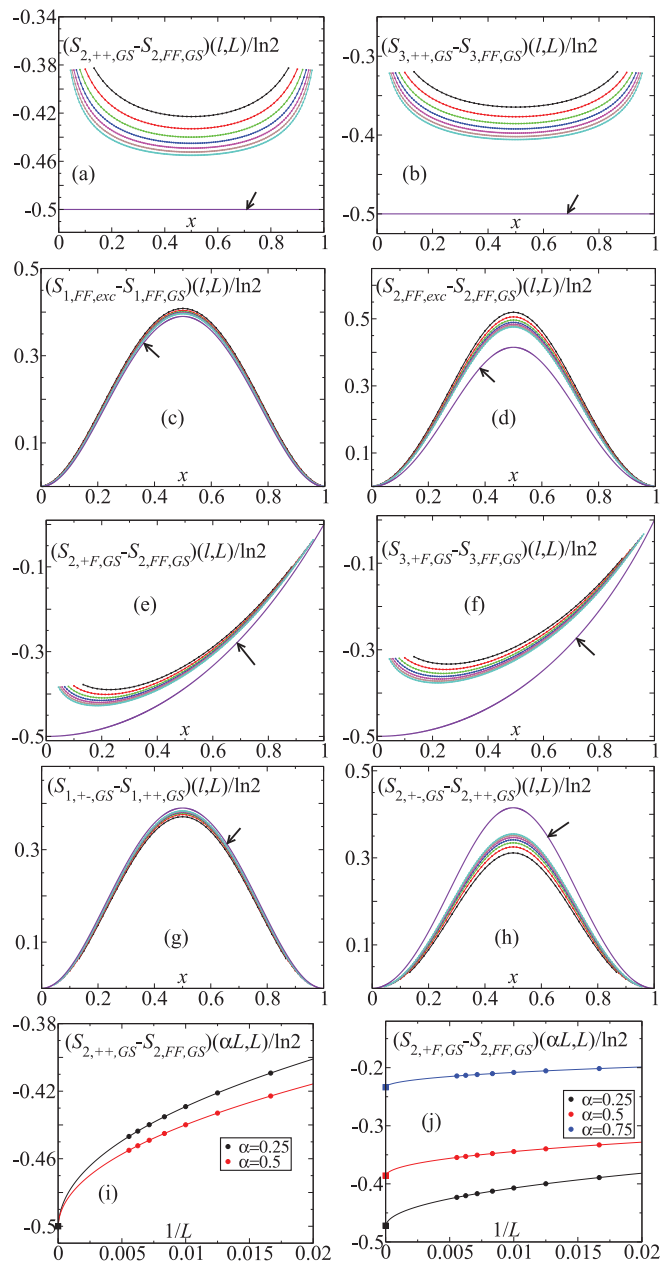


FIG. 1. (Color online) REE's in the 1D critical Ising model. (a)–(h) Black to turquoise (dotted lines),  $L = 60$ – $180$  numerical data; purple (solid line) + arrow, CFT predictions (the BE's are added to the CFT formulas when necessary). (i), (j) FSS relative to panels (a) and (e) (best fits use the five-parameters formula  $y = a_0 + a_1 x^{a_2} + a_3 x^{a_4}$ ; dots are numerical data; solid lines are best fits; squares are the CFT predictions).

Figures 1(c) and 1(d) show the convergence of the numerical results to the CFT prediction obtained with Eq. (12), for  $n = 1, 2$ .

We then consider the  $+FBC$ 's case. The fusion rule  $\mathcal{N}_{\mathbb{I},\sigma}^\sigma = 1$  implies that the spectrum contains just the conformal tower of the  $\sigma$  field, so the  $F$  function must be  $F_\sigma^{(n)}$ . The nontrivial fusion rule of the field  $\sigma$  yields different chiral correlators, which were computed for general  $n$  in Ref. 28. In our case, though, only a combination of them yields the appropriate

$F$  functions, which for  $n = 2, 3$  are given by

$$F_\sigma^{(2)}(x) = \cos \frac{\pi x}{4}, \quad F_\sigma^{(3)}(x) = \cos \frac{\pi x}{3}. \quad (13)$$

Figures 1(e) and 1(f) [also see Fig. 1(j)] display the DMRG results and the CFT predictions: the agreement, for  $L \rightarrow \infty$  is excellent, up to the constant term  $-\frac{1}{2} \ln 2$ .

Finally, we consider the  $+BC$  case (equivalent to the  $-+BC$  case). The spectrum contains just the conformal tower of the  $\chi$  operator, and therefore the REE's of the GS shall be the same as the ones of the first ES in the  $FFBC$  case [see Figs. 1(g) and 1(h)]. To conclude, we have shown that the CFT predictions for the Ising model with all possible conformal BC's agree with the numerical results, up to the constant contribution due to the BE.

(2) The second model is the  $c = 1$  compactified free boson. We shall next consider a massless free boson with a compactification radius  $R = 1$ . This CFT is rational, meaning that the chiral symmetry is enhanced in such a way that the number of primary fields is finite, and they have conformal dimensions  $h = 0, 1/8, 1/2, 1/8$ .<sup>4</sup> The corresponding conformal characters are given by setting  $\lambda = 0, 1, 2, 3 \pmod{4}$  ( $h_\lambda = \lambda^2/8$ ) in

$$K_\lambda(q) \equiv \frac{1}{\eta(q)} \sum_{n \in \mathbb{Z}} q^{\frac{1}{8}(4n+\lambda)^2}, \quad (14)$$

where  $\eta(q)$  is the Dedekind function. The conformal BC's are Dirichlet ( $D$ ) and Neumann ( $N$ ), and the corresponding boundary entropies are 0 and  $-\frac{1}{2} \ln 2$ .<sup>12</sup>

The lattice realization of this CFT is given by a spin-1/2 XX chain, with boundary couplings:<sup>29</sup>

$$H_B = - \sum_{j=1}^{L-1} (\sigma_j^x \sigma_{j+1}^x + \sigma_j^y \sigma_{j+1}^y) - \frac{1}{2} (\alpha_- \sigma_1^- + \alpha_+ \sigma_1^+ + \alpha_z \sigma_1^z + \beta_- \sigma_L^- + \beta_+ \sigma_L^+ + \beta_z \sigma_L^z), \quad (15)$$

where the  $DBC$ , on a given edge, is realized by setting all the boundary couplings to zero, while the  $NBC$  is realized, say on the left side, by choosing  $\alpha_z = 0$  and  $\alpha_+ = \alpha_- = 2$  (moreover, in the sermonic picture of the  $DDBC$ 's case, one has to work in the half-filled sector). The operator content of the various models described by the Hamiltonian Eq. (15) can be expressed in terms of the partition functions of a free boson with different BC's.<sup>12,29</sup> The  $DD$  and  $NN$  partition functions can be written in terms of the characters in Eq. (14):

$$Z_{DD}(q) = K_0(q) + K_2(q), \quad (16)$$

$$Z_{NN}(q) = K_0(q). \quad (17)$$

The absence of corrections for the GS in the  $DDBC$ 's case, with the exception of the usual oscillating ones,<sup>18</sup> has already been observed<sup>30</sup> and we confirm it numerically. We expect the same feature for the GS in the  $NNBC$ 's case, which we analyze with DMRG for system size  $L = 100$ , keeping up to 1100 states, using three sweeps and achieving a truncation error of  $10^{-10}$ . The results are shown in Figs. 2(a) and 2(b), for  $n = 2, 3$ : up to oscillating corrections, typical of  $c = 1$  systems, and the BE  $-\frac{1}{2} \ln 2$ , as expected from Eq. (9), we do not see any nonconstant correction.

We then consider the first ES with  $DDBC$ 's which, according to Eq. (16), is generated by a vertex operator

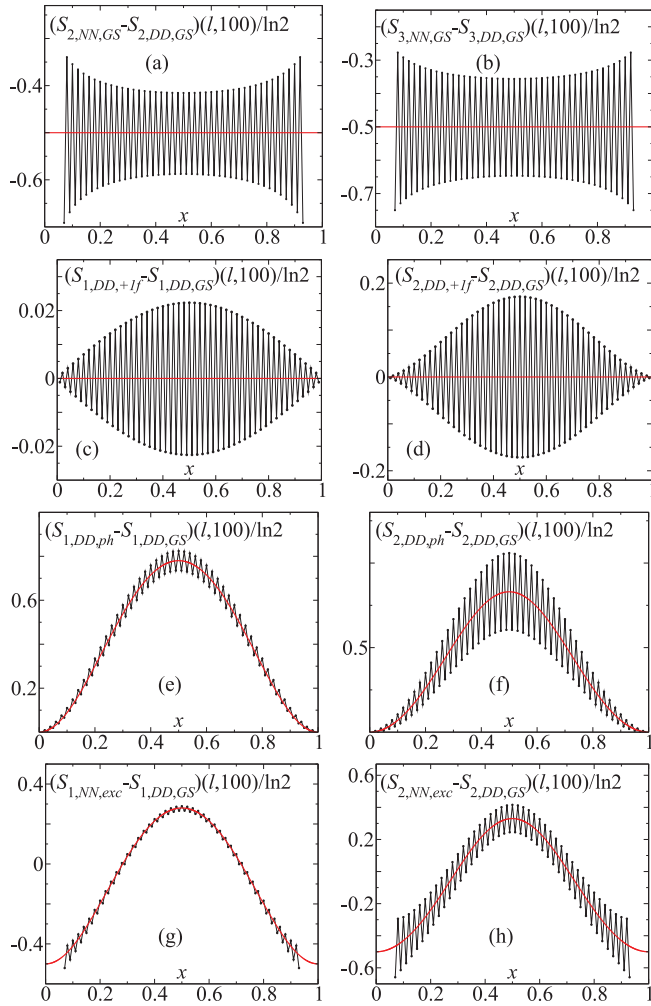


FIG. 2. (Color online) REE's in the model Eq. (15), part 1. Black dotted lines,  $L = 100$  numerical data; red solid line, CFT predictions (the BE's are added to the CFT formulas when necessary).

with conformal dimension  $1/2$ . The  $F_{\Upsilon}^{(n)}$  functions of vertex operators  $\Upsilon$  are equal to 1, for all  $n$ , so the REE's receive no corrections.<sup>9</sup> We verify this result by identifying this excitation in the fermionic version of the Hamiltonian Eq. (15) with the addition (or subtraction) of a fermion at half filling. Figures 2(c) and 2(d) show the  $n = 1, 2$  REE's for these states, which confirmed the absence of corrections.

For  $DD$  and  $NNBC$ 's, there is another ES, with conformal weight  $h = 1$ , associated to the primary field  $i\partial\phi$ . For  $DDBC$ 's it corresponds to the lowest particle-hole state created from the half-filled ground state;<sup>9,10</sup> in the  $NNBC$ 's case, there is no particle number conservation, so it is simply the first ES. In the former case, we use the method of Ref. 22, and in the latter we use the multitarget DMRG,<sup>31</sup> to compute the relative REE's, shown in Figs. 2(e)–2(h). Up to oscillations (and the BE in the  $NN$  case), we find excellent agreement with Eq. (12).

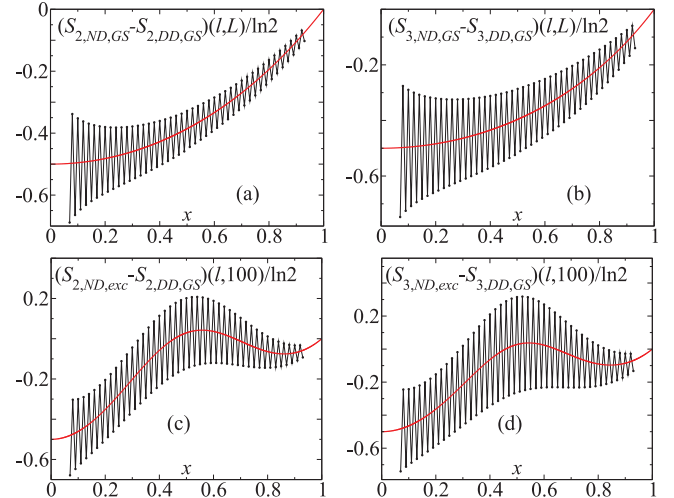


FIG. 3. (Color online) REE's in the model Eq. (15), part 2. See the caption of Fig. 2.

Finally, we study the  $NDBC$ 's case, whose partition function<sup>12</sup> cannot be written in terms of the characters (14). However, it can be shown that

$$Z_{ND}(q) = \chi_{1/16}(q)[\chi_0(q) + \chi_{1/2}(q)], \quad (18)$$

where  $\chi_{0,1/2,1/16}$  are the characters of the primary fields of the Ising model. Equation (18) implies that the operator content corresponding to  $NDBC$ 's is given by the tensor product of two Ising models. In particular, the GS is associated with the operator  $\mathbb{I} \otimes \sigma$ , resulting in the correction  $F_{\sigma}^{(n)}$ , and the first ES with  $\sigma \otimes \chi$ , resulting in the correction  $F_{\sigma}^{(n)} F_{\chi}^{(n)}$  (plus a BE contribution  $-\frac{1}{2} \ln 2$ ): we show in Fig. 3 the results for the  $n = 2, 3$ , obtained with multitarget DMRG, finding, even in this case, a remarkable agreement between CFT and numerics.

We conclude that, for the critical Ising and XX quantum spin chains under any conformal BC's, the REE's of the low-lying states are obtained, apart from the BE's and the oscillations, from the correlators of the primary operators of the underlying CFT: the finite-size behavior of the REE's of quantum chains with open boundaries identifies the primary operators in the CFT, providing, in principle, a tool for deepening the understanding of the operator content of a CFT.

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